

## Office of Energy Research

The Office of Energy Research (OER) within DOE supports basic investigations at NREL that provide fundamental knowledge of energy-related materials. Currently, basic energy research is conducted in materials sciences, chemical sciences, energy biosciences, and advanced energy projects.

DOE OFFICE OF ENERGY					
NREL Funding by Fiscal Year					
(\$ in millions--Budget Authority)					
	Fiscal Year*				
	FY1995	FY1996	FY1997	FY1998	FY1999
Office of Energy Research					
Operating					
Materials Sciences (KC02)	1.1	1.6	1.6	1.7	1.7
Chemical Sciences (KC03)	1.9	2.0	2.0	2.1	2.1
Advanced Energy Projects (KC05)	1.4	1.2	1.2	1.2	1.2
Energy Biosciences (KC06)	0.1	0.1	0.1	0.1	0.1
University & Science Education (KT)	0.3	0.1	0.1	0.1	0.1
Subtotal Operating	\$4.8	\$4.9	\$4.9	\$5.1	\$5.2
Capital Equipment (35KC)	0.4	0.4	0.4	0.4	0.4
Total Energy Research	\$5.2	\$5.3	\$5.3	\$5.5	\$5.7
Percent of Total Laboratory Funding	2%	3%	3%	3%	3%
*FY 1995 and FY 1996 are actuals; FY 1998 and beyond are projections in current-year dollars assuming 3% inflation.					

## Materials Science

NREL's fundamental materials studies are aimed at developing new classes of advanced semiconductor material architectures and novel renewable energy processes such as photo-voltaics (PV) and photoelectrochemistry. Activities include development and application

of theories, semiconductor theory, specific studies on III-V PV materials and devices, and measurement and modeling of opto-electronic and II-VI materials.

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NREL conducts cutting-edge fundamental research in materials science and solid-state theory to support various renewable energy technologies. The Laboratory's role is to strengthen basic research

that is the source of fundamental new ideas that drive technology and innovation. NREL plans to continue developing and maintaining state-of-the-art capabilities.

Planned materials science research activities during the next 5 years include:

- Solid-state theory work, including: 1) developing a thermodynamic theory for certain alloys (i.e., Si/GaP) to predict the phase diagram and phase transitions, 2) studies on electronic properties of transition metal alloys, and 3) prediction of band gaps in semiconductor configurations
- Growth of novel-ordered semiconductor alloys by organometallic chemical vapor deposition and molecular beam epitaxy, characterization of their opto-electronic properties, development of theoretical methodology to study ordering phenomena, and correlation with experimental results
- Studies on composition modulation in III-V superlattice structure that leads to some unique materials and device architecture
- Growth, characterization, and theory of structurally tolerant electronic oxides for photovoltaic and related applications
- Computer-aided predictions of energetics and thermodynamics of light metal alloys for automotive applications

These activities focus on continued growth of interactive research and development (R&D) with industrial partners through vigorous pursuit of work-for-others contracts and cooperative research and development agreements. Technology transfer activities will be strengthened in more mature technological areas.

## ***Chemical Sciences***

NREL performs basic research in all relevant areas of photoconversion to demonstrate the scientific feasibility of using solar light energy to produce fuels and chemicals in direct conversion processes. Basic research in this area is necessary before applied R&D programs can be initiated to develop technology for transfer to U.S. industry.

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Photoconversion encompasses all quantum-conversion processes other than photovoltaics

that lead to the *direct* production of fuels and chemicals. Solar light energy, the driving force for photoconversion processes, can be used to convert simple substrates such as water, carbon dioxide, and nitrogen to hydrogen, alcohol, and ammonia using photobiological, photochemical, photoelectrochemical, and catalytic processes. A broad array of other products are possible.

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Conversion efficiencies of 5%-10% (solar to hydrogen) are currently obtainable in the laboratory; processes and devices must be 10%-30% efficient (depending on the exact approach) to meet future program goals. Theoretical efficiency limits are on the order of 50%-60%. Photoconversion, an area of fundamental research, is expected to lead to a

new generation of fuel- and chemical-producing renewable energy technologies.

NREL research involves photoelectrochemistry, interfacial photochemistry, liquid crystal synthesis and catalysis, photophysics and photochemistry, electrochromics, and photobiology activities. The ideas that NREL is pursuing represent the foundation for a new generation of renewable energy technologies and are a radical departure from current renewable energy programs.

Photoconversion activities help expand the nation's basic research foundation in areas that could contribute to solving global energy and environmental problems. Demonstration of the scientific feasibility of these approaches is expected to result in new applied and exploratory development programs for DOE's Office of Energy Efficiency and Renewable Energy (EE) after FY 2000, when current EE programs may be phased out, after successful technology transfer to industry.

NREL has expertise in several areas relevant to carbon dioxide recycling, a promising area of research. Here a scientist is synthesizing an inorganic catalyst used in the electrocatalytic reduction of carbon dioxide to methanol. (Photo - Warren Gretz, NREL)

Two photoconversion research areas that hold great promise are carbon dioxide recycling and artificial photosynthesis. The objective of the former is to develop a large-scale capability to recycle carbon dioxide by using it as a substrate for chemical or biological synthesis. For example, carbon dioxide could be converted to fuels and chemical feedstocks by chemical and microbial photosynthetic methods.

NREL is in a unique position to take the technical lead in this area based on ongoing research and technical expertise in electrochemical carbon dioxide concentration and reduction, microbial carbon dioxide fixation, and development of novel catalysts for conversion of carbon dioxide/carbon monoxide to chemical feedstocks. Although current research efforts are in the early stage of development, progress is being made in several areas. In 10 years, some of these concepts will be ready for more applied study and development. Examples might include oceanic carbon dioxide

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**Although basic research efforts are currently in early stages in artificial photosynthesis, significant progress is being made in several areas...**

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sequestration, microbial photosynthetic conversion to fuels and chemicals, and the synthesis of catalysts for light-driven electrochemical production of fuel (methanol or methane) and chemical feedstock intermediates (e.g., ethylene glycol).

Carbon dioxide recycling would help enhance environmental quality by mitigating the major greenhouse gas (carbon dioxide), resulting in reduced global warming. Development of these technologies is also expected to contribute to our international competitiveness in heavy industries and the chemical industry, the development of carbon dioxide as a virtually inexhaustible raw material for fuel and chemical feedstocks production, and a stable domestic fuel supply.

Artificial photosynthesis includes innovative photobiological, photochemical, and photoelectrochemical processes for renewable energy applications. Although basic research efforts are also currently in early stages, significant

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**NREL's efforts represent future technology that will help keep U.S. industry competitive with our trading partners.**

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progress is being made in several areas and in 10 years, some of these concepts will be ready for more applied study and development. Examples include advanced semiconductor-based photoconversion devices, the production of organic PV and photoelectrochemical systems for generating fuel and electricity, and molecular water-splitting devices.

Artificial photosynthesis represents a new area of applied research and development that is expected to lead to new generations of fuel- and chemical-producing renewable energy technologies, necessary to keep the United States in a strong competitive position in the worldwide energy markets of the future.

Artificial photosynthesis includes all types of photochemistry; here hydrogen is produced from water at over 10% solar conversion efficiency using a photoelectrochemical cell. (Photo - Warren Gretz, NREL)

Industrial interest in NREL's photoconversion activities is just beginning. Experience has shown that most of that interest has been from Japanese companies (due to the long-term nature of the research); therefore, a major effort will be made to seek out U.S. industrial partners to advise them of future opportunities, keep them informed about progress being made, and ensure their appropriate involvement in the work. NREL's efforts represent future technology that will help keep U.S.

industry competitive with our trading partners.

## ***Energy Biosciences***

There are many potential ways to use the energy of sunlight to generate fuels and chemicals directly from renewable resources using photoconversion processes. Examples include producing 1) hydrogen by photolyzing water molecules; 2) hydrocarbons, carbohydrates, and polymers by biological reduction of carbon dioxide; and 3) ammonia by biological nitrogen fixation.

In studying the biological photosystem that converts light into chemical energy, NREL uses mutant algal strains to split water and produce hydrogen in the photobioreactor pictured in the background. (Photo - Warren Gretz, NREL)

NREL's current research focuses on photosynthetic water-splitting, with emphasis on the biological photosystem that converts light into chemical energy and on the manganese/enzyme complex that uses the energy to catalyze the water-splitting process. Substantial progress has been made in characterizing the structure of the complexes and elucidating mechanisms by which they function using a number of biophysical, biochemical, genetic, and immunological approaches. Basic knowledge of the biological water-splitting

process may ultimately translate into natural or artificial water-splitting devices that can produce useful products.

## ***Advanced Energy Projects***

The Advanced Energy Projects Division (AEPD) funds innovative high-risk research projects that could lead to specific technology development within a 3-year period. The following NREL projects were funded by OER AEPD and are in various stages of completion:

- Hot-carrier solar cells
- PV-powered electrochromic "smart windows"
- Atomic-scale engineering of thermophotovoltaic semiconductors

Successful completion of these projects are expected to be followed by other high-risk projects, some of which are currently being reviewed for future funding.

## ***Integration of Basic Sciences with DOE Technology Programs***

- A high-efficiency photovoltaic project involving many of the national laboratories and several universities has been initiated under the umbrella of the U.S. DOE Center of Excellence for the Synthesis and Processing of Advanced Materials
- An integrated R&D project on photochemical solar cells based on dye-sensitized titanium oxide has been initiated jointly by OER/Chemical Science, OER/Advanced Energy Projects, and DOE/EE Office of Utility Technologies, Photovoltaics Division